

# 1-Perfluorobutanesulfonic acid

375-73-5 | DTXSID5030030

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2.70

Global applicability domain: Outside

Local applicability domain index: 4.19e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chlorothalonil</div> <div>Measured: 3.26</div> <div>Predicted: 3.11</div>	<div>Image not found</div> <div>Chloranil</div> <div>Measured: 2.32</div> <div>Predicted: 2.41</div>	<div>Image not found</div> <div>Sulfone, methyl pentafluorophenyl</div> <div>Measured: 1.46</div> <div>Predicted: 2.02</div>
<div>Image not found</div> <div>Tetrachlorophthalic acid</div> <div>Measured: 3.30</div> <div>Predicted: 3.30</div>	<div>Image not found</div> <div>Fthalide</div> <div>Measured: 3.30</div> <div>Predicted: 3.20</div>	